

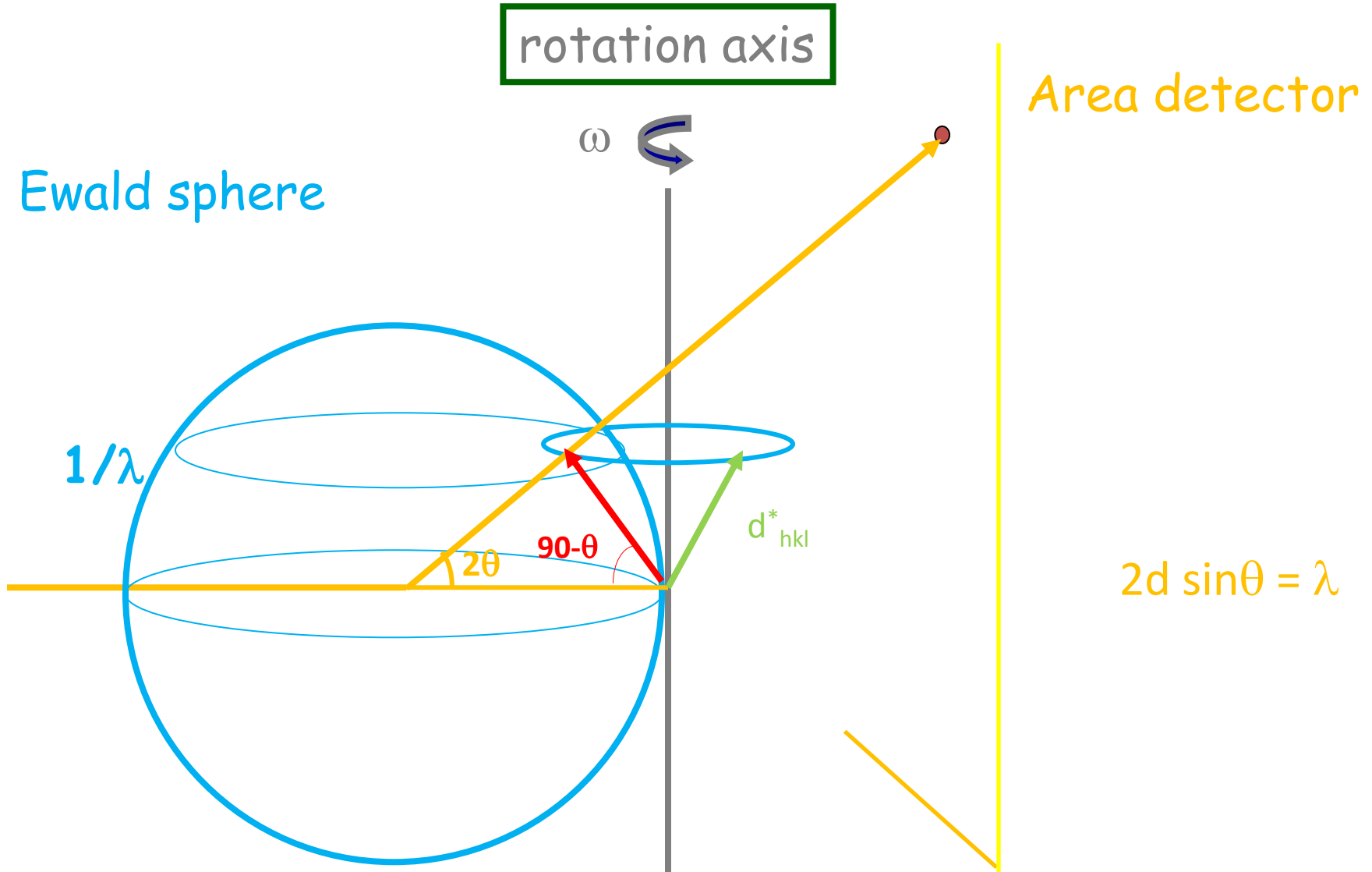
Eval15

A.M.M. Schreurs, X. Xian, L.M.J. Kroon-Batenburg,  
*J. Appl. Cryst.* (2010). **43**, 70-82.

# help

- Typing “help” will open a webpage with the manual.
- Typing “help commandname” will open a webpage with the manual entry for the commandname.  
Example: “help focus”

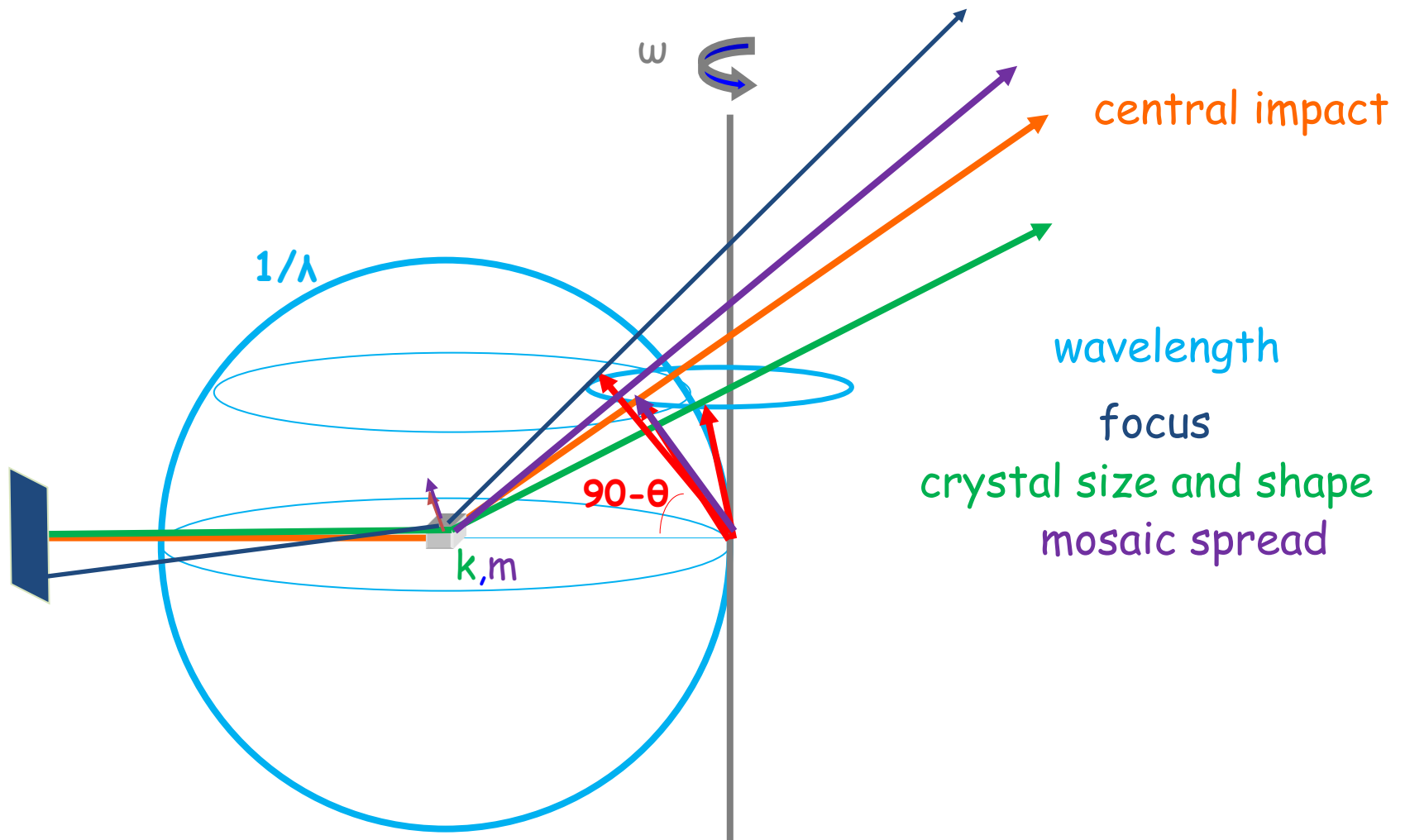
# Diffraction geometry



# General impact

$\omega$  rotation to Bragg condition at  $\zeta$ :

$$\cos \zeta = (\sin \theta - \sin \chi_{fk}) / (\cos \chi_{fk} \cos \chi)$$



# Least squares (SVD)

$$\chi^2 = \sum_{i=1}^N w_i \left[ \rho_i - JP_i - \sum_m^M J_m P_{im} - ax_i - by_i - c \right]^2$$

$$I = J \sum_{i=1}^N P_i$$

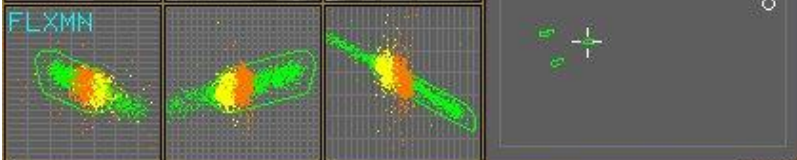
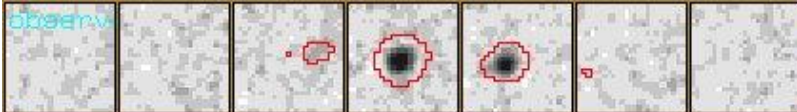
$$\sigma_i = \sqrt{\rho_i + bgnoise^2} \quad w_i = \frac{1}{\sigma_i^2}$$

Standard deviation of integrated reflection

$$\sigma_I^2 = \sigma_J^2 \left( \sum_{i=1}^N P_i \right)^2$$

$$fom_{box} = \left[ \frac{\sum_{i=1}^N w_i (\rho_i - \rho_i^{calc})^2}{N - N_p} \right]^{1/2}$$

Variances and co-variances available



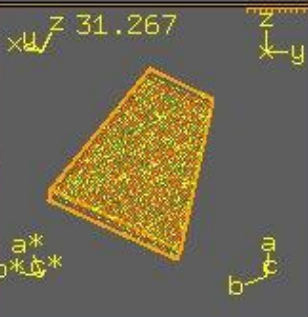
```
s02f001 102:-3 7 4
re,th,du 0.81 26.08 1.15
impact -12.10 -8.37 31.27
mosaic 0.30
volume 2895.00 1.00
shfinal -0.00 0.02 0.03
finalimp -12.10 -8.35 31.30
finalhkl -3.00 7.00 3.99
gravity -12.00 -8.27 31.14
restfrac 0.67 0.33
```

```
curr prev init
exhor -0.004 0.000 0.000
exver 0.024 0.000 0.000
exrot 0.028 0.000 0.000
```

```
simulate 10000
I sigma I/sig
Main 3069.24 82.25 37.31
EVAL14 2973.61 84.69 35.11
```

```
box peak bg
initfom 0.37 0.73 0.34
fom 0.35 0.46 0.34
initcor 0.97 0.98 0.21
cor 0.98 0.99 0.21
```

```
sim pix ins
Main 9954 224
Edge 46
```



# Configuration files

- detector.pic
- focus.pic
- refine.pic
- simulation.pic
- spectrum.pic
- crystal.pic
- mosaic.pic
- [eval15.init]



# Read boxfile

- The command “read” opens a boxfile
- Example:  
read 1 100  
opens the first boxfile  
reads reflection number 100  
displays the reflection graphically

# pq

- With the command “pq” the program will search for the next reflection with  $I/\sigma > 10$
- reflections with error flags (overflow, overlap, etc.) will be skipped

# Refinement variables

- The command “free” makes a variable refinable
- Example:  
free mosaic
- Only useful to determine parameters for the configuration files
- For the final intensity determination, use only free shextra

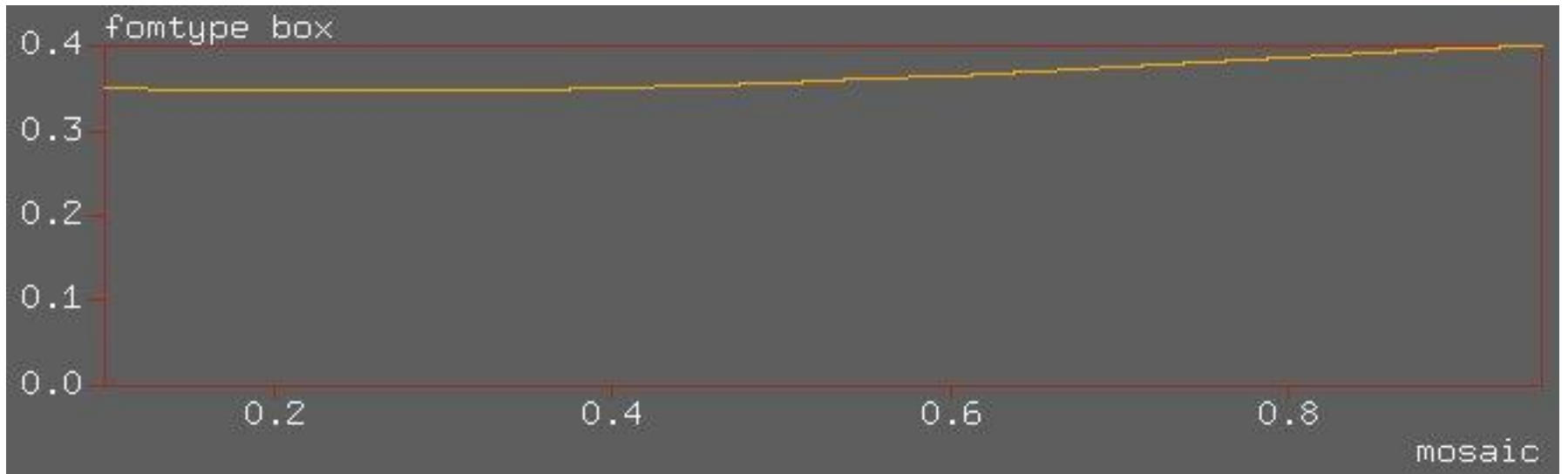
# refine

- With the command “refine” all free variables are refined
- Target function: fombox

# onescan

- The command “onescan” iterates a variable from startvalue to stopvalue
- Example:  
refine (to refine impact position)  
distribution type onescan  
distribution plot  
onescan mosaic 0.05 0.1 1.0  
(increment 0.05, startvalue 0.1, stopvalue 1.0)

# onescan



Minimum at mosaic = 0.25 for this reflection

# mosaic

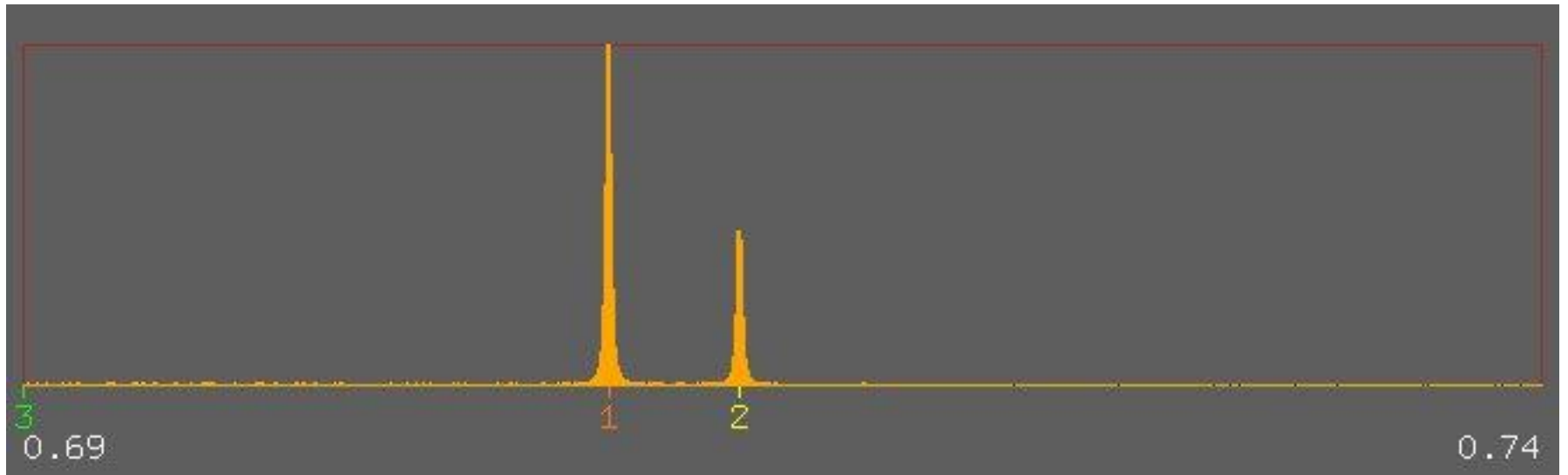
- The description of the mosaicity is given in the file mosaic.pic
  - Isotropic mosaicity
  - Anisotropic mosaicity (animo, anivec)
- With mosaicadd you can prepare a “mosaicity spectrum”
- The “mosaic spectrum” is a possibility to handle cracked crystals.

# spectrum

- The X-ray spectrum of the primary beam is described in the file spectrum.pic
- You can add additional wavelengths using the command “lamdaadd”
- The command “show lambda” prints the current values
- With “distribution type lambda” and “distribution plot” you obtain a graphical output.



# distribution plot

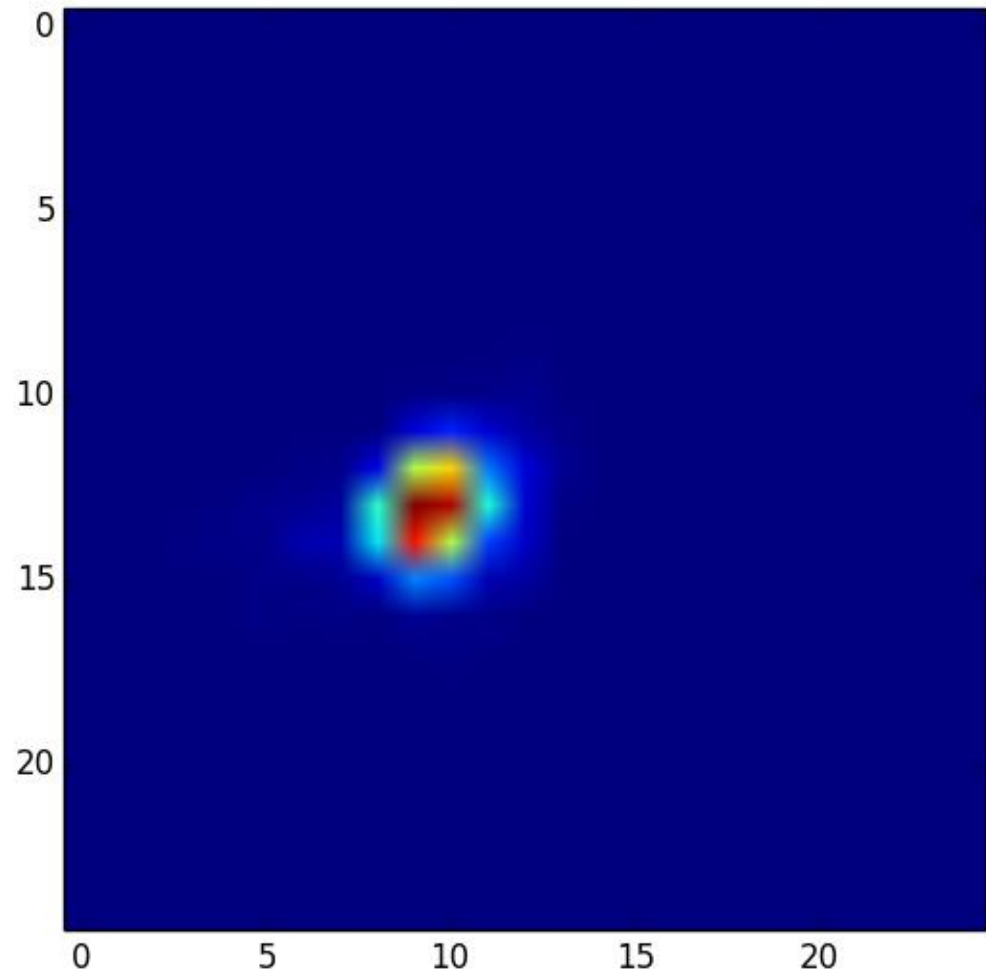


# printslices

- With the command “printslices” it is possible to print pixel intensities on the screen
- Example:  
printslices simulated on  
go
- With “slicewrite” you can write the pixel intensities to a file

# printslices

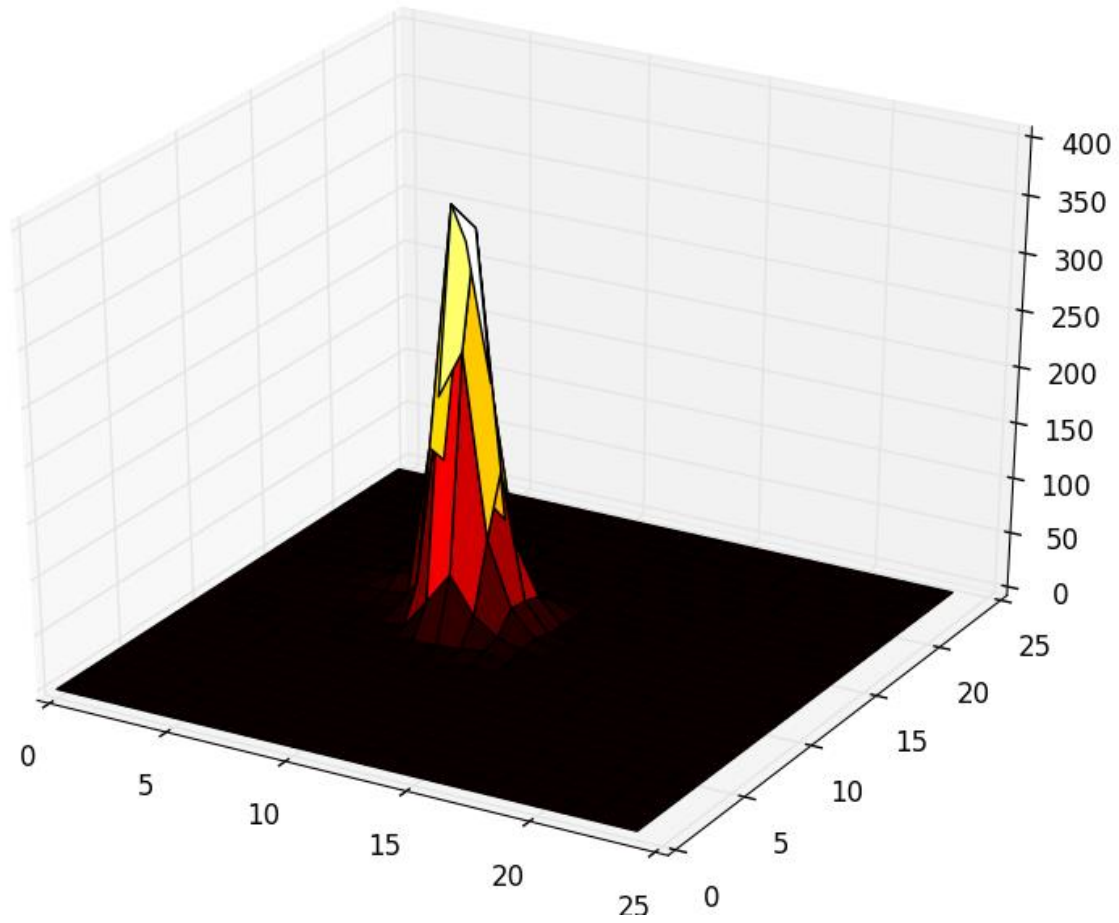
```
==== simulated ====
frame|
  5 | 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0 1 2 2 2 2 2 2
=====
25 |
24 |
23 |
22 |
21 |
20 |
19 |
18 |
17 |
16 |          1 2
15 |          2 2 4 7 1
14 |          1 29 58 26 11 4
13 |          2 4 33 205 249 87 29 6 1
12 |          2 5 6 10 147 364 348 140 27 2
11 |          2 4 4 17 17 128 325 206 67 23 1
10 |          1 3 4 7 22 93 75 17 11
  9 |          1 2 1 2 1 8 4 3
  8 |          1 2          1 1
  7 |          1
  6 |
  5 |
  4 |
  3 |
  2 |
  1 |
minimum 0.0 maximum 364.0 sum 2870.0 mean 4.592 sigma 30.661
```



simulated frame 5

hkl -3 7 4

s02f001.shoe 102



program "refl3d" (part of the Eval suite)